Wave-packet view of the Dirac electron

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By viewing the electron as a wavepacket in the positive energy spectrum of the Dirac equation, we are able to achieve a much clearer understanding of its behavior under weak electromagnetic fields. The intrinsic spin magnetic moment is found to be established from the self-rotation of the wavepacket. A non-canonical structure is also exhibited in the equations of motion due to non-Abelian geometric phases of the Dirac spinors. The wavepacket energy can be expressed simply in terms of the kinetic, electrostatic, and Zeeman terms only. This can be transformed into an effective quantum Hamiltonian by a novel scheme, and reproduces the Pauli Hamiltonian with all-order relativistic corrections.

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When the electron spin was first discovered, Uhlenbeck and Goudsmit regarded that it came from the self-rotation of the electron charge sphere[1]. However, this idea was soon swept off by Lorentz, who argued that the surface of sphere would rotate with a tangential speed at 137 times of the speed of light in order to produce the spin angular moment of $\hbar/2$[2]. One is thus forced to accept the spin as a discrete degree of freedom in abstract form, and eventually finds comfort in the Dirac theory[3], which explains the atomic spectra with great accuracy.

In the non-relativistic limit, the electron spin manifests through its physical attribute, an intrinsic magnetic moment, called the Bohr magneton. It is responsible for the Zeeman splitting of atomic spectral lines in a magnetic field. The spin also couples with orbital motion in the presence of an electric field, such as the Coulomb field inside an atom, which is responsible for the fine structures of the atomic spectra. Such effects are nicely captured in the Pauli Hamiltonian, which can be rigorously derived from the Dirac equation through the Foldy-Wouthuysen (FW) transformation[4]. However, the appearance of the intrinsic magnetic moment for the spin has been mysterious, and the usual physical picture linking the spin-orbit energy to the Zeeman effect has been rather cumbersome: A simple reference-frame argument misses a factor of two, and Thomas precession has to be taken into account to make the story complete[5].

In this paper, we take an alternative point of view to regard the electron as a wavepacket in the positive energy spectrum of the Dirac equation. The wavepacket has a minimum radius of the Compton wavelength, which is larger by a factor of 137 than the so-called classical radius of the electron, the size that Lorentz used in his argument. In our viewpoint, the wavepacket is found to be self-rotating, with an orbital angular momentum twice of the spin, and produces a magnetic moment of the Bohr magneton with its circulating charge. Therefore, the heuristic picture of Uhlenbeck and Goudsmit is essentially correct, and the so-called intrinsic magnetic moment of the spin originated from the orbital motion at the fundamental level.

In the presence of weak electromagnetic fields, it is possible to formulate a semiclassical dynamics for the variables of the center of charge, kinetic momentum and the average spin[6,7,8]. The magnetic moment gives the Zeeman term as a correction to the wavepacket energy, but the spin-orbit energy is notably absent. The spin-orbit term can arise only because of a shift from the physical position variable to an effective but unphysical variable in the Pauli Hamiltonian[9,10], which is closely related to the non-abelian geometric phase of the Dirac spinors[11]. In this work, we formulate a generalization of the Peierls substitution[12], which transforms the wavepacket energy to the Pauli Hamiltonian for arbitrary momenta[13] by a novel quantization procedure. In our treatment the spin-orbit coupling is a natural product in the canonicalization of the physical variables, and its form is found to be gauge dependent. We also suggest that, for a particle with anomalous magnetic moment, its mean position calculated from the expectation value of the position operator is actually not the true center of charge, and a correction term is required in predicting the correct trajectory of the particle.

We now proceed with the calculations leading to the above results. We first construct a wavepacket from the positive part of the energy spectrum[14,15],

$$|w\rangle = \int d^3\mathbf{q} a(\mathbf{q},t) e^{i\mathbf{q}\cdot\mathbf{r}} [\eta_1(\mathbf{q},t)|u_1\rangle + \eta_2(\mathbf{q},t)|u_2\rangle], \quad (1)$$

where η_i are the probability amplitudes of finding the electron in the two bands, and the Dirac electron wavepacket constitutes of linearly combination of spin up and spin down amplitudes of a free particle with a localized distribution function $a(\mathbf{q},t)$ centered at $\mathbf{q}_c$ in momentum space. The phase of $a(\mathbf{q},t)$ is chosen to ensure that the mean position of the wavepacket is located at $\mathbf{r}_c$. The conventional Dirac spinors $|u_i\rangle$ are obtained from a gauge rotation $e^{\beta\boldsymbol{\alpha}\cdot\hat{q}\omega/2}$ from $(1000)^T$ and $(0100)^T$, in which $\boldsymbol{\alpha}$ and β are the familiar Dirac matrices, and $\tan\omega = \frac{\hbar q}{mc}$.[16]

The intrinsic minimum size of electron wavepacket can be obtained by introducing the projection operators, P

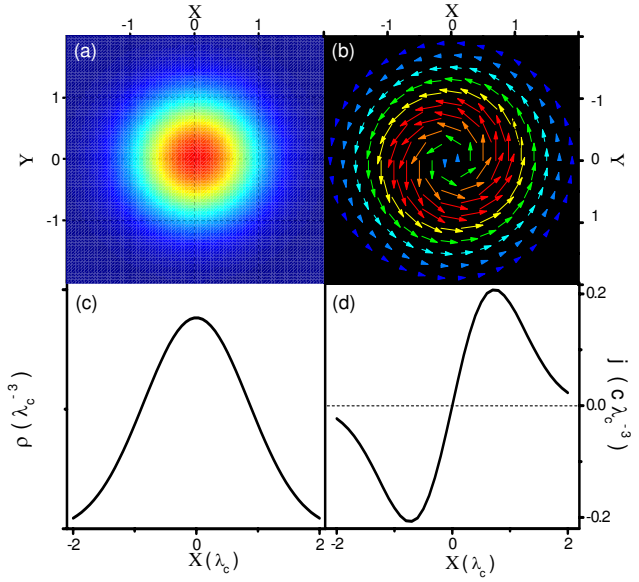

FIG. 1: (Color online) Distributions of (a) particle density $\rho = w^\dagger(\mathbf{r})w(\mathbf{r})$ and (b) particle current density $\mathbf{j}(\mathbf{r}) = w^\dagger(\mathbf{r})c\boldsymbol{\alpha}w(\mathbf{r})$ on the X-Y plane for an electron wavepacket, the spin is oriented out of the plane. The units are in λ_c. The colors indicate the magnitude of the density from low (blue) to high (red). The (c) and (d) are profiles of (a) and (b) along the X-axis.

and Q, for the electron and positron parts of the energy spectrum respectively, with $P+Q=1$. The mean square radius of the wavepacket can then be written as[17]

$$(\Delta r)^2 = \langle \mathbf{r}P\mathbf{r}\rangle - \langle \mathbf{r}\rangle^2 + \langle \mathbf{r}Q\mathbf{r}\rangle, \tag{2}$$

the wavefunction $|w\rangle$ is an eigenstate of P with eigenvalue 1. Using this fact, one can see that $\langle \mathbf{r}P\mathbf{r}\rangle - \langle \mathbf{r}\rangle^2$ is simply the mean squared radius for the projected position operator $P\mathbf{r}P$, and therefore is positive definite. The remaining part

$$\langle \mathbf{r}Q\mathbf{r}\rangle = \int d^3q|a(\mathbf{q})|^2\left[\frac{\lambda_c}{2\epsilon^2(q)}\right]^2 \tag{3}$$

is also positive definite, where the Compton wavelength $\lambda_c = \hbar/mc$ is involved and $\epsilon(q) \equiv \sqrt{1+(\hbar q/mc)^2}$. If we consider a wavepacket with a relatively sharp shape in momentum space, then $\langle \mathbf{r}Q\mathbf{r}\rangle^{1/2} = \frac{\lambda_c}{2\epsilon^2(q_c)}$, which reduces to $\lambda_c/2$ as $q_c \to 0$. This may be regarded as the intrinsic size of the non-relativistic electron. If one wishes to probe length scales smaller than the Compton wavelength, the positron spectrum must be involved in the wavepacket and therefore the physical entity being probed is no longer a pure electron.

Within this framework, the electron wavepacket is found to be rotating about its center of charge in general, and this rotation is responsible for the intrinsic magnetic moment usually associated with the spin. The Fig.1 shows the probability distribution and the current density of an electron wavepacket with a spin oriented out of the plane in the frame of wavepacket. An orbital circulation around the spin axis can be clearly seen from this figure. The mechanical angular momentum for the orbital circulation can be calculated from the formula $\mathbf{L} = m\langle(\mathbf{r}-\mathbf{r}_c)\times\mathbf{v}\rangle = m\int d^3r(\mathbf{r}-\mathbf{r}_c)\times\mathbf{j}(\mathbf{r})$. A general analytic formula for this quantity has been derived in Ref.[14], which has the following form $\mathbf{L} = \eta^\dagger\boldsymbol{\mathcal{L}}\eta$, where $\eta = (\eta_1,\eta_2)^T$ is a two-component spinor, and

$$\boldsymbol{\mathcal{L}}_{ij}(\mathbf{q}_c) = \sum_{l=3,4} m\langle u_i|i\frac{\partial}{\partial\mathbf{q}_c}|u_l\rangle\times\langle u_l|c\boldsymbol{\alpha}|u_j\rangle. \tag{4}$$

Notice that indices i and j refer to positive energy levels, where index l runs over the negative energy levels. A straightforward calculation of Eq. (4) yields

$$\boldsymbol{\mathcal{L}} = \frac{\hbar}{\epsilon^2}\left(\boldsymbol{\sigma} + \lambda_c^2\frac{\mathbf{q}_c\cdot\boldsymbol{\sigma}}{\epsilon+1}\mathbf{q}_c\right), \tag{5}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices. It can be shown that a natural connection exists between the self-rotating angular momentum and the projected spin,

$$\hbar\boldsymbol{\tau}_{ij}(\mathbf{q}_c) \equiv \hbar\langle u_i|\boldsymbol{\Sigma}|u_j\rangle = \epsilon\boldsymbol{\mathcal{L}}_{ij}(\mathbf{q}_c), \tag{6}$$

where $\boldsymbol{\Sigma}$ are 4×4 spin matrices. At extremely high velocity($\epsilon \to \lambda_c\mathbf{q}_c$), $\boldsymbol{\mathcal{L}}$ reduces to zero but $\boldsymbol{\tau}$ approaches the projection along the direction of momentum $(\hat{q}_c\cdot\boldsymbol{\sigma})\hat{q}_c$.

The magnetic moment of the wavepacket is similarly defined as $\mathbf{M} = -\frac{e}{2}\langle(\mathbf{r}-\mathbf{r}_c)\times\mathbf{v}\rangle = -\frac{e}{2}\int d^3r(\mathbf{r}-\mathbf{r}_c)\times\mathbf{j}(\mathbf{r})$. This differs from the mechanical angular momentum of self-rotation by the factor of $e/2$ in place of m, which ensures the usual relation $\mathbf{M} = -(e/2m)\mathbf{L}$ to be hold. One thus has

$$\mathbf{M} = -\frac{ge}{2\epsilon m}\frac{\hbar\boldsymbol{\tau}}{2}, \tag{7}$$

where $g=2$. It is very interesting to see that the so-called intrinsic magnetic moment of the spin really comes from the self-rotation of the wavepacket. In this sense, Uhlenbeck and Goudsmit's view of the electron spin as a rotating sphere is meaningful. The sphere is rigid near the core in the sense that the rotation velocity of the wavepacket is approximately proportional to the radius near the center.

The spin magnetic moment also appears naturally in the energy of the wavepacket when a magnetic field is present. In the Dirac Hamiltonian, the magnetic field enters only through the vector potential, and there is not a Zeeman energy term. By expanding the vector potential about the center of the wavepacket, we find the wavepacket energy up to first order in the gradients as[14,18],

$$E(\mathbf{r}_c,\mathbf{k}_c) = E_0(k_c) - e\phi(\mathbf{r}_c) + \frac{e}{2mc}\mathbf{L}(\mathbf{k}_c)\cdot\mathbf{B}, \tag{8}$$

where $\mathbf{k}_c \equiv \mathbf{q}_c + \frac{e}{c}\mathbf{A}(\mathbf{r}_c)$, $\mathbf{A}$ is the vector potential, and $E_0(k_c) = \epsilon(k_c)mc^2$. The Zeeman energy in Eq. (8) is just

the gradient correction in the wavepacket energy. It is strikingly observed that there does not exist a spin-orbit coupling in the wavepacket energy, which one would normally think to be present to first order in the electric field. It turns out that the semiclassical dynamics of the Dirac electron is non-canonical, and spin-orbit coupling is deeply rooted in the Berry-curvature field which specifies this non-canonical structure. By requiring the wavepacket to satisfy the time-dependent Dirac equation, one can derive the effective Lagrangian[14],

$$L_{eff} = i\hbar\eta^\dagger\frac{\partial\eta}{\partial t}+\hbar\dot{\mathbf{k}}_c\cdot\mathbf{R}+\hbar\mathbf{k}_c\cdot\dot{\mathbf{r}}_c-\frac{e}{c}\mathbf{A}\cdot\dot{\mathbf{r}}_c-E(\mathbf{r}_c,\mathbf{k}_c), \quad (9)$$

where $\mathbf{R}$ is the Berry connection based on the gauge specified below Eq. (1), $\mathbf{R} = \frac{\lambda_c^2}{2\epsilon(\epsilon+1)}\ \mathbf{k}_c\times\langle\boldsymbol{\sigma}\rangle$, in which $\langle\boldsymbol{\sigma}\rangle \equiv \eta^\dagger\boldsymbol{\sigma}\eta$. The equations of motion for the center of charge position and momentum, correct to linear order in fields, then follow as

$$\hbar\dot{\mathbf{k}}_c = -e\mathbf{E}-\frac{e}{c}\frac{\hbar\ \mathbf{k}_c}{\epsilon m}\times\mathbf{B}, \quad (10)$$

$$\dot{\mathbf{r}}_c = \frac{\hbar\mathbf{k}_c}{\epsilon m}+\frac{e}{\hbar}\left(\mathbf{E}\times\mathbf{F}+\ \mathbf{B}\cdot\mathbf{F}\frac{\hbar\mathbf{k}_c}{\epsilon mc}\right), \quad (11)$$

the Berry curvature $\mathbf{F} = -\frac{\lambda_c^2}{2\epsilon^3}\left(\langle\boldsymbol{\sigma}\rangle+\lambda_c^2\frac{\mathbf{k}_c\cdot\langle\boldsymbol{\sigma}\rangle}{\epsilon+1}\mathbf{k}_c\right)$. These equations need to be solved in conjunction with the equation for spin precession,

$$\langle\dot{\boldsymbol{\sigma}}\rangle = \frac{e}{\epsilon mc}\left[\mathbf{B}+\frac{\mathbf{E}\times\hbar\ \mathbf{k}_c}{(\epsilon+1)mc}\right]\times\langle\boldsymbol{\sigma}\rangle, \quad (12)$$

which agrees with the BMT equation[19]. The equations of motion, Eqs. (10),(11), and (12), are all invariant under SU(2) gauge transformation.

The same equations of motion have been obtained from a formal semiclassical expansion to first order in $\hbar$[6], which is not surprising because our dimensionless weak-field parameters are $eE\lambda_c/mc^2$ and $eB\lambda_c/mc^2$, which are both proportional to the Planck constant. Our results are not limited to low momenta and become even more accurate for high momenta where the energy gap is greater. For example, one can obtain the semiclassical but relativistic cyclotron frequency ω_c when the electron is confined in a plane perpendicular to the magnetic field (say $\mathbf{E}=0$), $\omega_c = eBc/E(k_c)$, where $E(k_c) = E_0(k_c)+e/(2mc)\ \mathbf{L}\cdot\mathbf{B}$ is the total energy of the electron.

It is evident from the equations of motion that the position and momentum of the wavepacket do not form a canonical pair, due to the presence of the gauge potentials $\mathbf{R}$ and $\mathbf{A}$. Quantization of the non-canonical equations of motion for the semiclassical Dirac electron presents an interesting and important physics problem[6,20]. If one can find new variables $\mathbf{r}$ and $\mathbf{p}$, such that the effective Lagrangian is of the following form,

$$L_{eff} = i\hbar\eta^\dagger\frac{\partial\eta}{\partial t}+\ \mathbf{p}\cdot\dot{\mathbf{r}}-E(\mathbf{r},\mathbf{p}), \quad (13)$$

then $\mathbf{r}$ and $\mathbf{p}$ would naturally be a classical canonical pair. To linear order of the fields (and up to total time derivatives), this is indeed possible by the transformation,

$$\mathbf{r} = \mathbf{r}_c-\mathbf{R}(\mathbf{k}_c)-\mathbf{G}(\mathbf{k}_c);$$
$$\mathbf{p} = \hbar\mathbf{k}_c-\frac{e}{c}\mathbf{A}(\mathbf{r}_c)-\frac{e}{2c}\mathbf{B}\times\mathbf{R}(\mathbf{k}_c), \quad (14)$$

where $G_\alpha \equiv 1/2(\partial\mathbf{R}/\partial k^\alpha)\cdot(\mathbf{R}\times\mathbf{B})$. Conversely, one can write

$$\mathbf{r}_c = \mathbf{r}+\mathbf{R}(\boldsymbol{\pi})+\mathbf{G}(\boldsymbol{\pi}),$$
$$\hbar\mathbf{k}_c = \boldsymbol{\pi}+\frac{e}{c}\mathbf{B}\times\mathbf{R}(\boldsymbol{\pi}), \quad (15)$$

where $\boldsymbol{\pi} = \mathbf{p}+\frac{e}{c}\mathbf{A}(\mathbf{r})$. This is entirely analogous to the Peierls substitution for the momentum variable. Naively, one expects the familiar presence of the gauge potentials, $\mathbf{R}$ and $\mathbf{A}$, to the position and momentum. However, this is not enough in this semiclassical formulation and extra corrections are required. The $\mathbf{G}$-term would further shift the position operator, but does not influence the velocity (to linear order in fields); similarly, the $\mathbf{B}\times\mathbf{R}$-term would shift the momentum, but does not alter the force.

One can *re-quantize* the semiclassical Dirac energy by promoting $\mathbf{r}$ and $\mathbf{p}$ in Eq (8) to be quantum conjugate variables, and $\langle\boldsymbol{\sigma}\rangle$ in the same equation to be Pauli matrices. The result turns out to be precisely the (relativistic) Pauli Hamiltonian accurate to all orders of the velocity (μ_B is the Bohr magneton)[13],

$$H(\mathbf{r},\mathbf{p}) = \epsilon(\pi)mc^2-e\phi(\mathbf{r})+\frac{\mu_B}{\epsilon(\epsilon+1)mc}\boldsymbol{\pi}\times\boldsymbol{\sigma}\cdot\mathbf{E}+\frac{\mu_B}{\epsilon}\boldsymbol{\sigma}\cdot\mathbf{B} \quad (16)$$

That is, one can obtain an effective quantum Hamiltonian by obtaining the semiclassical energy first, followed by using the (generalized) Peierls substituion for re-quantization. We emphasize that one would fail to reproduce the correct Pauli Hamiltonian if the extra corrections in Eq. (15) were not included. This alternative approach is simpler and more intuitive when compared to formal procedures of block-diagonalization, such as the Foldy-Wouthuysen transformation.

In Eq. (16), the spin-orbit coupling emerges from the first-order gradient expansion of the scalar potential, $\partial\phi/\partial\mathbf{r}\cdot\mathbf{R}$. This reveals a deep connection between the spin-orbit interaction and the non-canonical structure of the semiclassical Dirac theory. It must be remembered that the position variable $\mathbf{r}$ in the Pauli Hamiltonian does not correspond to the true position $\mathbf{r}_c$ of the Dirac electron. The former is sometimes called the mean position, but it is not really the mean position of the wave packet. In the literature, $-e\mathbf{R}$ has often been called an electric dipole[10], which couples to the electric field to give rise to the spin-orbit energy[11]. This is unfortunately artificial, because its existence depends on an unphysical assignment of the electron position, which depends on the choice of the SU(2) gauge. Indeed, the equations of motion based on the Pauli Hamiltonian is consistent with the Dirac theory if and only if one recognizes this fact.

If the Dirac particle has an anomalous magnetic moment (AMM), which may be originated from the coupling with quantized electromagnetic field, or from the internal motion of the constituent quarks in a nucleon, then in addition to the energy in Eq. (8), the semiclassical particle acquires an extra energy ($a \equiv g/2-1$),

$$\begin{aligned} E_{\rm AMM} &= a\mu_B \langle w|\beta(-i\boldsymbol{\alpha}\cdot\mathbf{E}+\boldsymbol{\Sigma}\cdot\mathbf{B})|w\rangle \\ &= a\mu_B\left[\frac{\mathbf{k}_c\times\langle\boldsymbol{\sigma}\rangle\cdot\mathbf{E}}{\lambda_c^{-1}\epsilon}+\left(\langle\boldsymbol{\sigma}\rangle-\frac{(\mathbf{k}_c\cdot\langle\boldsymbol{\sigma}\rangle)\mathbf{k}_c}{\lambda_c^{-2}\epsilon(\epsilon+1)}\right)\cdot\mathbf{B}\right] \end{aligned} \tag{17}$$

Unlike the energy in Eq. (8), the spin-orbit coupling is now explicit from the very beginning. It indicates that, when the particle has a AMM, the true center of charge $\mathbf{r}_c'$ has been further displaced from $\mathbf{r}_c$. In order to obtain the spin-orbit interaction in Eq. (17), the amount of displacement has to be $\mathbf{R}' = a(\lambda_c^2/2\epsilon)\ \mathbf{k}_c\times\langle\boldsymbol{\sigma}\rangle$. Indeed, if one replaces the $\mathbf{r}_c$ and $e/(2mc)$ in Eq. (8) with $\mathbf{r}_c' = \mathbf{r}_c+\mathbf{R}'$ and $eg/(4mc)$, then the AMM energy of the wavepacket can be fully reproduced from the simpler semiclassical energy in Eq. (8). Furthermore, following the same re-quantization scheme using the generalized Peierls substitution, one can indeed obtain the (relativistic) Pauli Hamiltonian with the exact AMM terms (Eq. (33) in Ref.[13]).

We emphasize that, since one expects no electric dipole from a point particle, the presence of the electric dipole energy indicates that the theory is only an effective one, and the position of the particle in the effective theory should differ from the true position by a Berry connection. Of course, in predicting the trajectory of the point particle, one always has to refer to its true position. Therefore, in the Dirac theory with $H_{\rm AMM} = a\mu_B\beta(-i\boldsymbol{\alpha}\cdot\mathbf{E}+\boldsymbol{\Sigma}\cdot\mathbf{B})$, the true position $\mathbf{r}$ is conjectured to be $\mathbf{r}_D+\mathbf{R}_D$, where $\mathbf{r}_D$ is the usual position operator, and $\mathbf{R}_D = (a\mu_B/e)(-i\beta\boldsymbol{\alpha})$ is the displacement required to generate the electric field term in $H_{\rm AMM}$. The displacement (Berry connection) is originated from the projection of a larger state space (for example, the one that includes the quantized electromagnetic field) to the Hilbert space of the relativistic particle. Thus, the true velocity operator of the particle should be,

$$\dot{\mathbf{r}}_D+\dot{\mathbf{R}}_D = (1+a)c\boldsymbol{\alpha}-a\beta\frac{\boldsymbol{\pi}}{m}+a^2\frac{\mu_B}{mc}\left(\mathbf{E}\times\boldsymbol{\Sigma}+\gamma_5\mathbf{B}\right). \tag{18}$$

The magnitude of the anomaly a for an electron is of the order of 10^{-3} and might be too small for such a difference to be observed. However, the anomaly for a nucleon is of order one. Therefore, it is possible to observe and verify such a deviation in experiments using relativistic proton beams.[21]

In summary, we demonstrate an alternative method to investigate the Dirac electron by semiclassical wavepacket approach which provides a much more intuitive and pedagogic picture of the Dirac electron. In this framework, the intrinsic size of the non-relativistic electron is of the order of λ_c, and the self-rotation motion generates a magnetic moment equals precisely the conventional spin magnetic moment. The dynamics of the wavepacket is also studied and reveals a direct link between the Berry connection and the spin-orbit coupling. By re-quantizing the semiclassical Dirac theory through a generalized Peierls substitution, we recover the relativistic Pauli Hamiltonian to all orders of velocity.

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